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A T-matrix approach for morphological characterization of spherical nanoparticles using laser

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Abstract A laser based setup is designed to study the morphological characteristics of spherical PbS nanoparticles. Polarized light from a diode laser is detected, after getting scattered from nanosized particulate matter, by analyzer mounted photodiodes placed angularly. The signals from the detectors are interfaced to a high resolution data acquisition system. The size and shape characterization is attempted using the computational T-matrix approach. The investigation is aimed at accurate and *in-situ* measurement of stable and unstable nanoparticulate matter.

Keywords T-matrix, diode laser, polarized light, nanoparticulate matter

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1. Introduction

The light scattering behavior of spherical particulate matter presents numerous theoretical and experimental challenges [1]. The surface morphology, along with the geometrical shape of the scattering particle, is the most important factor in determining the optical properties of such scatterer [2, 3]. There are various methods available to compute light scattering by spherical particulate matter. Waterman's T-matrix method, based on the linearity of Maxwell's equations, is widely used for such calculations. In T-matrix approach both the incident and the scattered fields $E^{inc}(\mathrm{R})$ and $E^{sca}(\mathrm{R})$ are expanded in vector spherical harmonics M_{mn} and N_{mn} as:

$$E^{inc}(\mathrm{R}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[a_{mn}\mathrm{RgM}_{mn}(k\mathrm{R}) + b_{mn}\mathrm{RgN}_{mn}(k\mathrm{R})\right]. \tag{1}$$

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$$E^{sca}(R) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[p_{mn} M_{mn}(kR) + q_{mn} N_{mn}(kR)\right], R > R_{>} \tag{2}$$

where, $k = 2\pi/\lambda$ is the wavenumber, λ is the wavelength in the surrounding medium Owing to the linearity of Maxwell's equations and boundary conditions, the relation between the scattered field coefficients p_{mn} and q_{mn} on the one hand and the incident field coefficients a_{mn} and b_{mn} on the other hand must be linear and is given by a transition (or Transition matrix) T as follows (Waterman, 1971) :

$$p_{mn} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n} \left[T^{11}_{\mathrm{mnm'n'}} a_{m'n'} + T^{12}_{\mathrm{mnm'n'}} b_{m'n'}\right] \tag{3}$$

$$q_{mn} = \sum_{n'=1} \sum_{m'=-n'} \left[T^{21}_{\mathrm{mnm'n'}} a_{m'n'} + T^{22}_{\mathrm{mnm'n'}} b_{m'n'}\right. \tag{4}$$

In compact matrix notation eqs. (3) and (4) can be rewritten as

$$= T \qquad \begin{matrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{matrix} \tag{5}$$

The above equation forms the basis of the **T-matrix** approach [4, 5, 6].

2. Experimental details

The schematic diagram of the experimental setup is shown in Figure 1. The setup consists of diode laser source (Melles Griot), controlled sample holders, photodetector arrangements

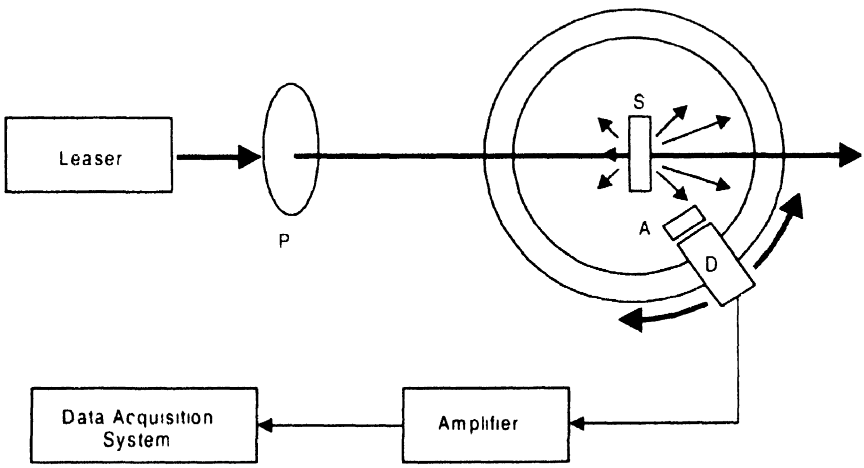

Figure 1. Outline diagram of light scattering experiment setup. Notation. P, Polarizer; S, Sample; D, AlGaAs photodiode.

data acquisition systems and associated instrumentation. Light beam from a diode laser (Red, λ = 635 nm, 3 mW) passes through a linear polarizer (Melles Groit, dia. 25mm). The polarizer placed in a rotating mount with a vernier dial is used to select either the perpendicular or parallel polarization component of the laser beam for using in the experiment. The laser light is scattered by a sample of nanoparticles at the centre of the circular disc. The scattered light intensity is sensed by the scattering detector (AlGaAs photodiode, RLD-78MA) with large sensing area connected to high gain, low noise OPAMP (LM 301AN) circuit. The photodiode detector can be rotated about an axis perpendicular to the plane of the circular disc. An analyzer optimized for the diode laser wavelength is used to determine the state of polarization of the scattered light after it reaches the detector. The whole set up is covered by a black polished metallic enclosure and beam stops are placed at points of strong intensity to minimize the intensity of stray reflections [7].

The light scattering experiment is carried out on large semiconductor PbS nanoparticles (>60nm) specially fabricated *via* chemical route [8, 9]. The experiments are carried out in differential mode, that is, scattered light intensity is initially measured from blank PVA matrix which does not have embedded nanoparticles and then measurements are made of the light intensity scattered from PVA matrix having embedded nanoparticles. The data obtained is then plotted and compared with theoretically generated T-matrix plot for particles of the same size, shape, refractive index and also for the same wavelength (632.8 nm).

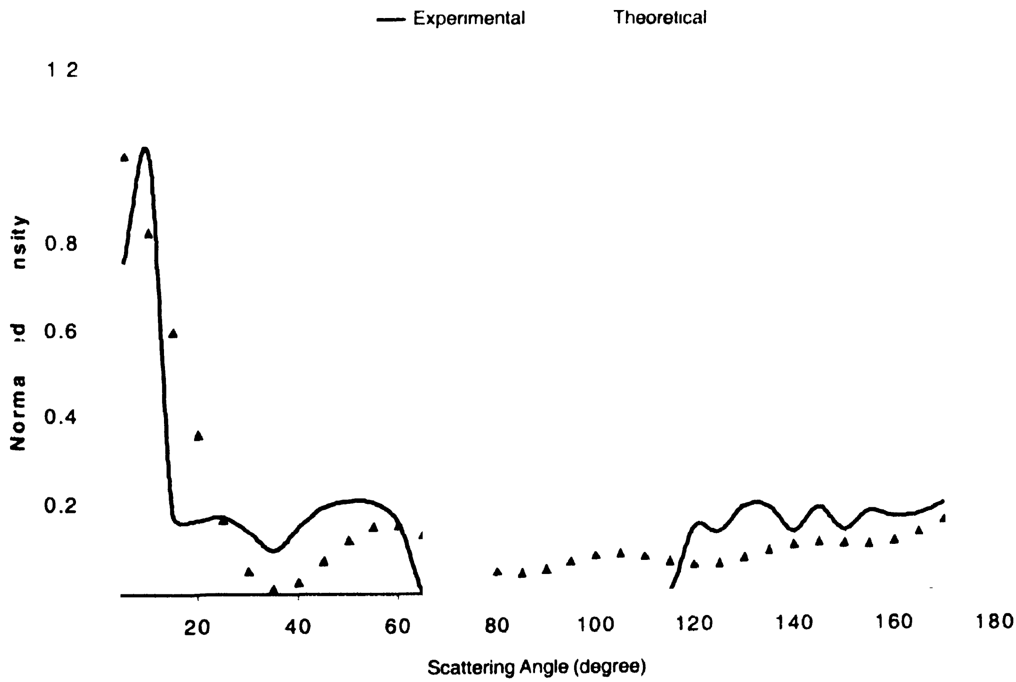

Figure 2. Angle *vs* scattered intensity.

3. Results and discussion

The attempt at designing and fabricating a highly efficient and economic setup for investigation of nanoparticles is carried out successfully First data is acquired, given in Figure 2, by the system for PbS nanoparticles embedded in PVA Subsequently an attempt is made to analyze the data using T-matrix formulation given in equations (1)–(4) For this, theoretical curves are generated for particles of all radii starting from 30 – 100 nm in steps of 5 nm Each theoretical curve is then compared with the curve for experimental data When there is an agreement between the two curves, we can ascertain that the experimental data is due to particles of radii corresponding to the theoretical curve Preliminary analysis shows that the size of the nanoparticles embedded in the polymer matrix has reached a size of around 60 to 70 nanometers

4. Conclusion

The setup has been found to be considerably accurate to a very high resolution The use of Diode laser and RLD-78MA photodiode has made the setup highly compact and energy efficient Moreover the initial attempt at data analysis using computational techniques is found to be an efficient method as the size of the nanoparticles calculated are in very good agreement with the transmission electron micrograph

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